

SIMULATION OF HEAVY ION REACTIONS WITH NONLOCAL KINETIC EQUATIONS

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Abstract

The incorporation of realistic trajectories of two-particle scattering into existing BUU or QMD codes meets considerable difficulties. We propose a method of replacing the scattering event by a tractable non-local scenario reproducing the correct asymptotics. The first principle derivation justifies the use of corresponding nonlocal kinetic equations. The nonlocal shifts are necessary if the system should approach an equation of state with second quantum virial coefficient. The modifications of QMD and BUU codes are discussed and comparison are presented with recent data. We find a pre-equilibrium production of particles leading to higher energetic distributions of protons.

1 Introduction

Recent dynamical simulations of heavy ion reactions at low and mid energies are based either on BUU or QMD simulations. These equations simulate the Boltzmann equation (BE) with the extension of Pauli-blocking and meanfield drift

$$\begin{aligned} \frac{\partial f_1}{\partial t} + \frac{\partial \varepsilon_1}{\partial k} \frac{\partial f_1}{\partial r} - \frac{\partial \varepsilon_1}{\partial r} \frac{\partial f_1}{\partial k} = \sum_b \int \frac{dp dq}{(2\pi\hbar)^3} \frac{1}{\mu^2} \frac{d\sigma}{d\Omega} \delta(\varepsilon_1 + \varepsilon_2 - \varepsilon_3 - \varepsilon_4) \\ \times [f_3 f_4 (1 - f_1)(1 - f_2) - (1 - f_3)(1 - f_4) f_1 f_2]. \end{aligned} \quad (1)$$

The arguments of distributions f and energies ε are shortened as $f_1 \equiv f_a(k, r, t)$, $f_2 \equiv f_b(p, r, t)$, $f_3 \equiv f_a(k - q, r, t)$, and $f_4 \equiv f_b(p + q, r, t)$, with momenta k, p, q , coordinate r , time t , spin and isospin a, b and reduced mass μ .

While the motion due to nonlinear meanfield is governed by the quasiclassical Hamilton equations for chosen test particles or wave packets, the collision is performed randomly if the particles meet inside the area of cross section or at the closest approach. By random choice of transfer momenta and averaging

over many runs the scattering probability given by the cross section in the Boltzmann equation is reproduced. Medium effects are discussed in terms of density and temperature dependent depletion of cross section.

However, there are modifications of the Boltzmann equation which have a more fundamental meaning. It has been noticed that the starting Boltzmann equation has an inherent contradiction. While the collision probability describes a finite diameter the collision takes place at a time instant and local in space. This deficiency has to be cured. Simple cases like hard sphere gases have been discussed already by Enskog [1] and in nuclear matter by Malfliet [2] and Halpert [3]. Resonance scattering has been discussed by Pratt and Danielewicz [4]. The aim of these corrections are to describe a realistic scattering event within kinetic theory in a way that the correct asymptotics are reproduced. Only by this way the virial corrections, e.g. the two-particle correlation energy in balance equations can be expected to be approached during time evolution. The original Boltzmann equation and consequently the standard BUU and QMD simulations lead to no binary correlation energy. As it was shown [5] this binary correlation can be reproduced within a non-local collision integral.

The need for nonlocal corrections can be stimulated by discussing the scattering of two particles as superpositions of wave packets [6] and similar [7]. The solution of the free Schroedinger equation can be written for the relative motion with c.m. momentum k as

$$\phi(p, k, t) = F(p, k) e^{-iE_p t} \quad (2)$$

and the asymptotic wave after scattering can be decomposed into $\Psi = \phi + \phi^{\text{sc}}$ with the scattered wave for large distance x from scattering center

$$\phi^{\text{sc}}(x, k, t) = \int \frac{dp}{(2\pi\hbar)^3} \mathcal{F}(p, k) \frac{f(p, \cos(px))}{x} e^{i(px - E_p t)} \quad (3)$$

with the scattering amplitude $f(p, \cos(px))$. We proceed now and expand the scattering amplitude around the center of mass momentum k

$$\begin{aligned} f(p, \cos(px)) &= |f(p, \cos(px))| e^{i\delta(p, \cos(px))} \\ &= f(k, \cos(kx)) \left(1 + (p - k) \nabla_p |f(p, \cos(px))|_{p=k} \right) e^{i(p-k) \nabla_p \delta(p, \cos(px))_{p=k}}. \end{aligned} \quad (4)$$

The derivative of the phase δ leads now to the definition of the effective space shifts Δ and the time shift Δ_{\parallel}

$$2\Delta = \nabla_p \delta = \partial_k \delta + \frac{\frac{x}{|x|} - \cos(xk) \frac{k}{|k|}}{|k|} \partial_{\cos(xk)} \delta \equiv \frac{k}{m} \Delta_{\parallel} + \Delta_{\perp} \quad (5)$$

where we denoted the shifts corresponding to the direction of k as \parallel and \perp . Expanding in (3) also $E_p = p^2/m = k^2/m + (p - k)2k/m$ and collecting all terms we obtain

$$\phi^{\text{sc}}(x, k, t) = \frac{f(k, \cos(kx))}{x} \int \frac{dp}{(2\pi\hbar)^3} \tilde{\mathcal{F}}(p, k) e^{ip(x+2\Delta-ut)} e^{-i\frac{k^2}{m}(\Delta_{\parallel}-t)} \quad (6)$$

where the wave packet velocity is $u = 2k/m$. We observe three effects of scattering on the asymptotics: (i) a genuine time delay Δ_{\parallel} , (ii) an effective displacement of the two colliding particle of Δ with respect to the center of mass and (iii) a modification of scattering probability $\tilde{\mathcal{F}} = \mathcal{F}(1 + (p - k)\nabla_p |f(p, \cos(px))|_{p=k})$.

In this contribution we will put these ideas of nonlocalities on the firm ground using the quantum kinetic equation with nonlocal scattering integrals which was derived from quantum statistics [5, 8] to show how the effect of nonlocalities play a role in simulations of heavy ion reactions and compare them with experiment.

2 Nonlocal kinetic equation

In [6, 5, 8] we have given a systematic derivation of nonlocal kinetic equation (NKE) which includes hard sphere like corrections, resonance like corrections as well as rotational angle corrections, which turned out to be important for angular momentum conservation. This kinetic equation completes all balance equations on the level of quantum second virial coefficients. The NKE-equation with the collected gradient terms reads $[\Delta_r = \frac{1}{4}(\Delta_2 + \Delta_3 + \Delta_4)]$

$$\begin{aligned} & \frac{\partial f_1}{\partial t} + \frac{\partial \varepsilon_1}{\partial k} \frac{\partial f_1}{\partial r} - \frac{\partial \varepsilon_1}{\partial r} \frac{\partial f_1}{\partial k} = \sum_b \int \frac{dpdq}{(2\pi)^5} \delta(\varepsilon_1 + \varepsilon_2 - \varepsilon_3 - \varepsilon_4 + 2\Delta_E) \\ & \times z_1 z_2 z_3 z_4 \left(1 - \frac{1}{2} \frac{\partial \Delta_2}{\partial r} - \frac{\partial \bar{\varepsilon}_2}{\partial r} \frac{\partial \Delta_2}{\partial \omega} \right) \\ & \times |T_{\text{sc}}^R|^2 \left(\varepsilon_1 + \varepsilon_2 - \Delta_E, k - \frac{\Delta_K}{2}, p - \frac{\Delta_K}{2}, q, r - \Delta_r, t - \frac{\Delta_t}{2} \right) \\ & \times [f_3 f_4 (1 - f_1)(1 - f_2) - (1 - f_3)(1 - f_4) f_1 f_2] \end{aligned} \quad (7)$$

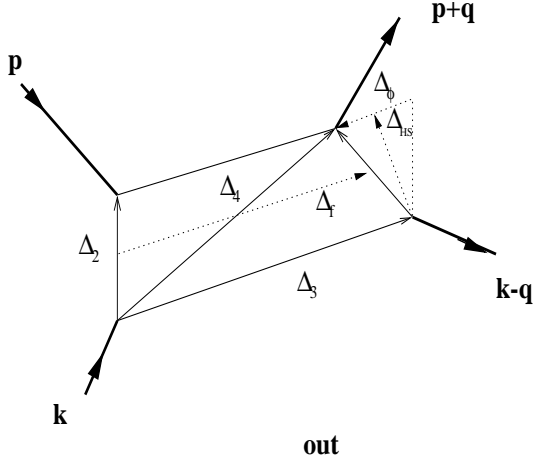


Figure 1: The equivalent scattering event of two colliding particles.

with the nonlocal shifts given as derivatives of the total phase shift of the scattering T -matrix $\phi = \text{Im} \ln T_{sc}^R(\Omega, k, p, q, t, r)$,

$$\begin{aligned} \Delta_2 &= \left(\frac{\partial \phi}{\partial p} - \frac{\partial \phi}{\partial q} - \frac{\partial \phi}{\partial k} \right) & \Delta_3 &= -\frac{\partial \phi}{\partial k} & \Delta_4 &= -\left(\frac{\partial \phi}{\partial k} + \frac{\partial \phi}{\partial q} \right) \\ \Delta_t &= \frac{\partial \phi}{\partial \Omega} & \Delta_E &= -\frac{1}{2} \frac{\partial \phi}{\partial t} & \Delta_K &= \frac{1}{2} \frac{\partial \phi}{\partial r}. \end{aligned} \quad (8)$$

After derivatives, Δ 's are evaluated at the energy shell $\Omega \rightarrow \varepsilon_3 + \varepsilon_4$. Unlike in (1), the subscripts denote shifted arguments: $f_1 \equiv f_a(k, r, t)$, $f_2 \equiv f_b(p, r - \Delta_2, t)$, $f_3 \equiv f_a(k - q - \Delta_K, r - \Delta_3, t - \Delta_t)$, and $f_4 \equiv f_b(p + q - \Delta_K, r - \Delta_4, t - \Delta_t)$.

The Δ 's are effective shifts and they represent mean values of various nonlocalities of the scattering integral as demonstrated in figure 1. These shifts enter the scattering integral in the form known from the theory of gases [1, 9, 10], however, the set of shifts is larger due to the medium effects on the binary collision that are dominated by the Pauli blocking of the internal states of the collision.

Now we want to use these derived nonlocalities to mimic the real scattering event in simulations. To this end we use a classical analogy of these nonlocalities and the scattering event as demonstrated by picture 1. We obtain the following scenario: Two particles approach until they reach a distance Δ_2 . Then they form a molecule traveling over a distance Δ_f with a time Δ_t . During this propagation the molecule rotate about Δ_ϕ . Now the kinetic equation (7) is numerically tractable by recent Monte Carlo or BUU codes [11] as demonstrated below.

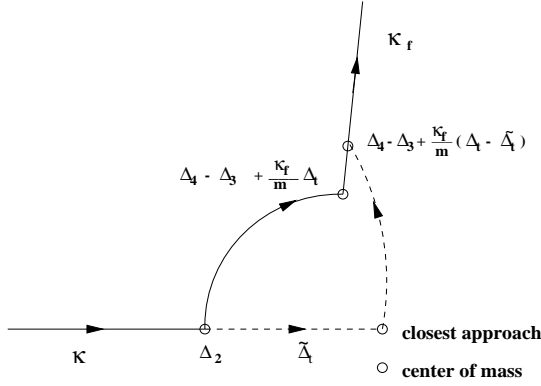


Figure 2: A nonlocal binary collision (solid line) together with the scenario of sudden jump at the closest approach.

3 Instant approximation

The selfconsistent evaluation of all Δ 's for all collisions would be too demanding. We employ two kinds of additional approximations. First, following approximations used within the BUU equation, we neglect the medium effect on binary collision, i.e., use the well known free-space T-matrix. Second, we rearrange the scattering integral into an instant but non-local form. This instant form parallels hard-sphere-like collisions what allow us to employ computational methods developed within the theory of gases [12] similarly as it has been done in [11].

In the instant approximation we let particles to make a sudden jump at time t from r_a and r_b to effective final coordinates \tilde{r}_a and \tilde{r}_b . These effective coordinates and momenta $\tilde{\kappa}$ and \tilde{K} are selected so that at time $t + \Delta_t$ particles arrive at the correct coordinates, r'_a and r'_b , with the correct momenta, κ' and K' . Accordingly, in the asymptotic region, after $t + \Delta_t$, there is no distinction between the non-instant and instant pictures, which is shown as solid line in figure 2. This asymptotic condition is naturally met if one extrapolates the out-going trajectories from known coordinates and momenta at $t + \Delta_t$ back to the time t . Doing so one finds that the effective coordinates read

$$\tilde{r}_a = r'_a - \frac{k - q}{m} \Delta_t = r_a + \Delta_3 - \frac{k - q}{m} \Delta_t, \quad (9)$$

$$\tilde{r}_b = r'_b - \frac{p + q}{m} \Delta_t = r_b + \Delta_4 - \Delta_2 - \frac{p + q}{m} \Delta_t. \quad (10)$$

When incorporating the displacements into the QMD simulation code, we have to face the fact that two particles are selected for a collision if they meet

at the point of closest approach. This distance is different from the distance Δ_2 required from the equivalent scattering scenario presented in figure 2 as solid line. We consider now the time required to travel from Δ_2 to the distance of closest approach $\tilde{\Delta}_t = \frac{m}{2\kappa^2}\kappa\Delta_2$ in analogy to [13]. Within this scenario we are allowed to jump at the point of closest approach to the final asymptotics (9) and (10) with the additional distance the particle travel during $\tilde{\Delta}_t$. The effective final coordinates thus have to be evaluated as

$$\tilde{r}_{a,b} = \frac{R_a + R_b}{2} \mp \Delta, \quad (11)$$

with the effective displacement

$$\Delta = \frac{1}{2}\Delta_2 - \Delta_3 + \frac{k - q}{m}(\Delta_t - \tilde{\Delta}_t). \quad (12)$$

Since the center of mass does not jump in the collision, the final displacement can be also written in an alternative way, $\Delta = \frac{1}{2}\Delta_2 + \Delta_4 - \Delta_2 - \frac{p+q}{m}(\Delta_t - \tilde{\Delta}_t)$. The non-local corrections are thus performed as follows. When the collision is selected, we evaluate Δ from (12) and (8), redisplay particles into \tilde{r}_a and \tilde{r}_b and continue with the simulation.

Let us note that from (8) and (12) the already presented shift (5) follows as it should.

At this point it is possible to establish a connection of the present theory to the hard-sphere-like corrections used by Malfliet [2] and Kortemeyer, Daffin and Bauer [11]. For hard spheres of the diameter d , the phase shift has a classical limit $\phi = \pi - |q|d$ which gives $\Delta_3 = 0$ and $\Delta_2 = \Delta_4 = \frac{q}{|q|}d$. The displacement thus has the same amplitude d for all binary collisions and points in the direction of the transferred momentum, as it is known from the Enskog equation [1].

4 Results for Simulation

In order to investigate the effect of non-local shifts on realistic simulations of a heavy ion reaction, we have evaluated Δ^f from the two-particle scattering T-matrix T^R in the Bethe-Goldstone approximation [14, 5] using the separable Paris potential [15]. The comparison of the shifts calculated for different potentials concerning partial wave coupling up to D-waves can be found in [16]. We have incorporated these shifts into a QMD code for the central collision of $^{129}\text{Xe} \rightarrow ^{119}\text{Sn}$ at 50 MeV/A.

Figure 3a shows the exclusive proton spectra subtracting the protons bound in clusters. This procedure is performed within a spanning tree model which is

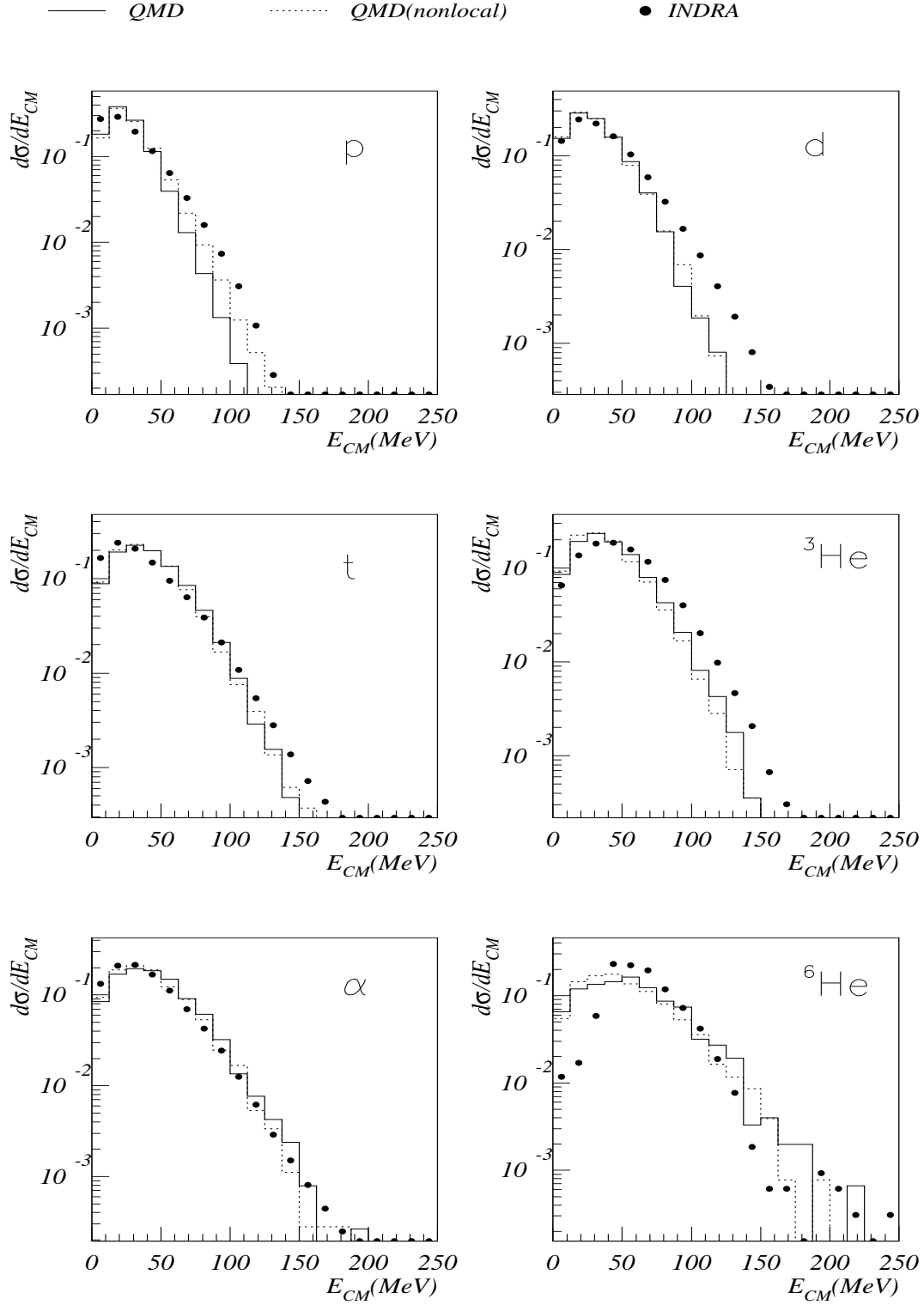


Figure 3: The particle spectra for central collision of $^{129}\text{Xe} \rightarrow ^{119}\text{Sn}$ at 50 MeV/A with and without non-local corrections. The data are extracted from recent INDRA experiments [17]. The non-local corrections bring the spectrum of the protons towards the experimental values leaving the clusters almost unchanged.

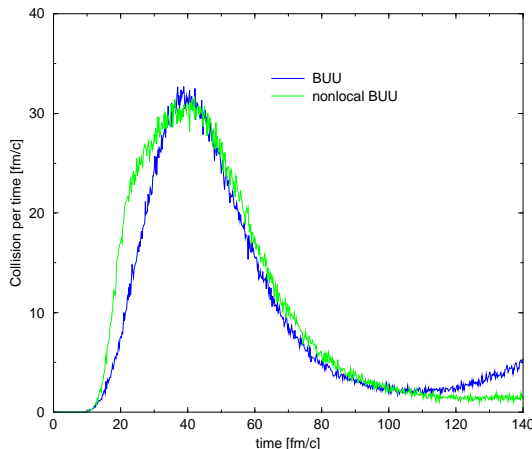


Figure 4: The number of collisions per time with and without non-local collisions within a BUU simulation of the same reaction as in figure (3).

known to describe a production of light charged cluster in a reasonable agreement with the experimental data, Figs. 3b-f. Within the local approximation, however, the remaining distribution of high-energy protons is too low to meet the experimental values. As one can see, the inclusion of non-local collisions corrects this shortage of the QMD simulation. As demonstrated in Fig. 3, productions of light clusters are rather insensitive to the non-local corrections. This also shows that the improvement of the proton production is not on cost of worse results in other spectra.

A microscopic mechanism leading to the increase in the high-energy part of the particle spectrum can be traced down to an enhancement of the number of collisions at the pre-equilibrium stage of the heavy ion reaction demonstrated in Fig. 4 for the BUU simulation of the same reaction. This enhancement gives rise to an immediate proton production which itself translates into a high energetic spectra. In other words, the strong production of the high-energy protons follows from the pre-equilibrium emission of particles. The BUU simulation also shows that non-local corrections are important namely in the early stage of reaction well before most of light clusters are formed. It explains why the production of protons is affected while the formation of light clusters is nearly untouched by the non-local corrections.

5 Conclusion

In summary, as documented by the improvement of the high-energy proton production, the non-local treatment of the binary collisions brings a desirable contribution to the dynamics of heavy ion reactions. According to an experi-

ence from the theory of gases, one can also expect a vital role of non-localities in the search for the equation of state of the nuclear matter. It is encouraging that the non-local corrections are easily incorporated into the BUU and QMD simulation codes and do not increase computational time. Corresponding programs can be obtained from authors.

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